

Traditional and emerging perfluoroalkyl substances in the Cape
Fear River Watershed, North Carolina: Occurrence and fate
during conventional and advanced water treatment processes

Supporting Information

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Supporting information includes 4 tables and 3 figures.

Table S1. perfluoroalkyl substances (PFASs) detected in the Cape Fear River (CFR) watershed

Compound	Molecular weight	Formula	CAS #	# of perfluorinated carbons	Chain length (including all C, O and S)
Perfluorocarboxylic acids (PFCAs)					
Perfluorobutanoic acid (PFBA)		C ₄ HF ₇ O ₂	375-22-4	3	4
Perfluoropentanoic acid (PFPeA)		C ₅ HF ₉ O ₂	2706-90-3	4	5
Perfluorohexanoic acid (PFHxA)		C ₆ HF ₁₁ O ₂	307-24-4	5	6
Perfluoroheptanoic acid (PFHpA)		C ₇ HF ₁₃ O ₂	375-85-9	6	7
Perfluorooctanoic acid (PFOA)		C ₈ HF ₁₅ O ₂	335-67-1	7	8
Perfluorononanoic acid (PFNA)		C ₉ HF ₁₇ O ₂	375-95-1	8	9
Perfluorodecanoic acid (PFDA)		C ₁₀ HF ₁₉ O ₂	335-76-2	9	10
Perfluorosulfonic acids (PFSAs)					
Perfluorobutane sulfonic acid (PFBS)		C ₄ HF ₉ SO ₃	29420-49-3	4	5
Perfluorohexane sulfonic acid (PFHxS)		C ₆ HF ₁₃ SO ₃	355-46-4	6	7
Perfluorooctane sulfonic acid (PFOS)		C ₈ HF ₁₇ SO ₃	111873-33-7	8	9
Perfluoroalkyl ether carboxylic acids with one ether group (mono-ether PFECAs)					
Perfluoro-2-methoxyacetic acid (PFMOAA)		C ₃ HF ₅ O ₃	674-13-5	2	4
Perfluoro-3-methoxypropanoic acid (PFMOPrA)		C ₄ HF ₇ O ₃	377-73-1	3	5
Perfluoro-4-methoxybutanoic acid (PFMOBA)		C ₅ HF ₉ O ₃	863090-89-5	4	6
Perfluoro-2-propoxypropanoic acid (PFPrOPrA)		C ₆ HF ₁₁ O ₃	13252-13-6	5	7
Perfluoroalkyl ether carboxylic acids with multiple ether group (multi-ether PFECAs)					
Perfluoro(3,5-dioxahexanoic) acid (PFO2HxA)		C ₄ HF ₇ O ₄	39492-88-1	3	6
Perfluoro(3,5,7-trioxaoctanoic) acid (PFO3OA)		C ₅ HF ₉ O ₅	39492-89-2	4	8
Perfluoro(3,5,7,9-tetraoxadecanoic) acid (PFO4DA)		C ₆ HF ₁₁ O ₆	39492-90-5	5	10

Figure S1. Molecular structures of PEFCAs in this study

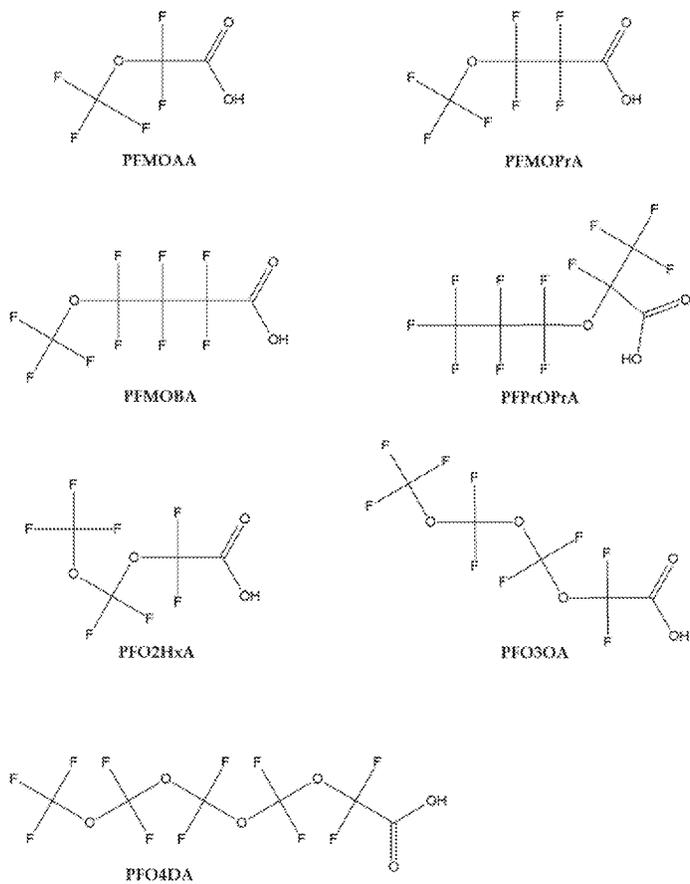


Table S2. LC gradient method for PFAS analysis

Time (min)	Mobile Phase A% (v/v)	Mobile Phase B%	Flow Rate (mL/min)
0 – 2	95	5	0.9
2 – 5	95	5	0.9
5 – 10	95 → 10	5 → 90	0.9
10 – 10.1	10	90	0.9
10.1 – 14	10 → 95	90 → 5	0.9

Mobile phase A: 2 mM ammonium acetate in ultrapure water with 5% methanol

Mobile phase B: 2 mM ammonium acetate in acetonitrile with 5% ultrapure water

Table S3. LC Gradient Method for PFAS Analysis

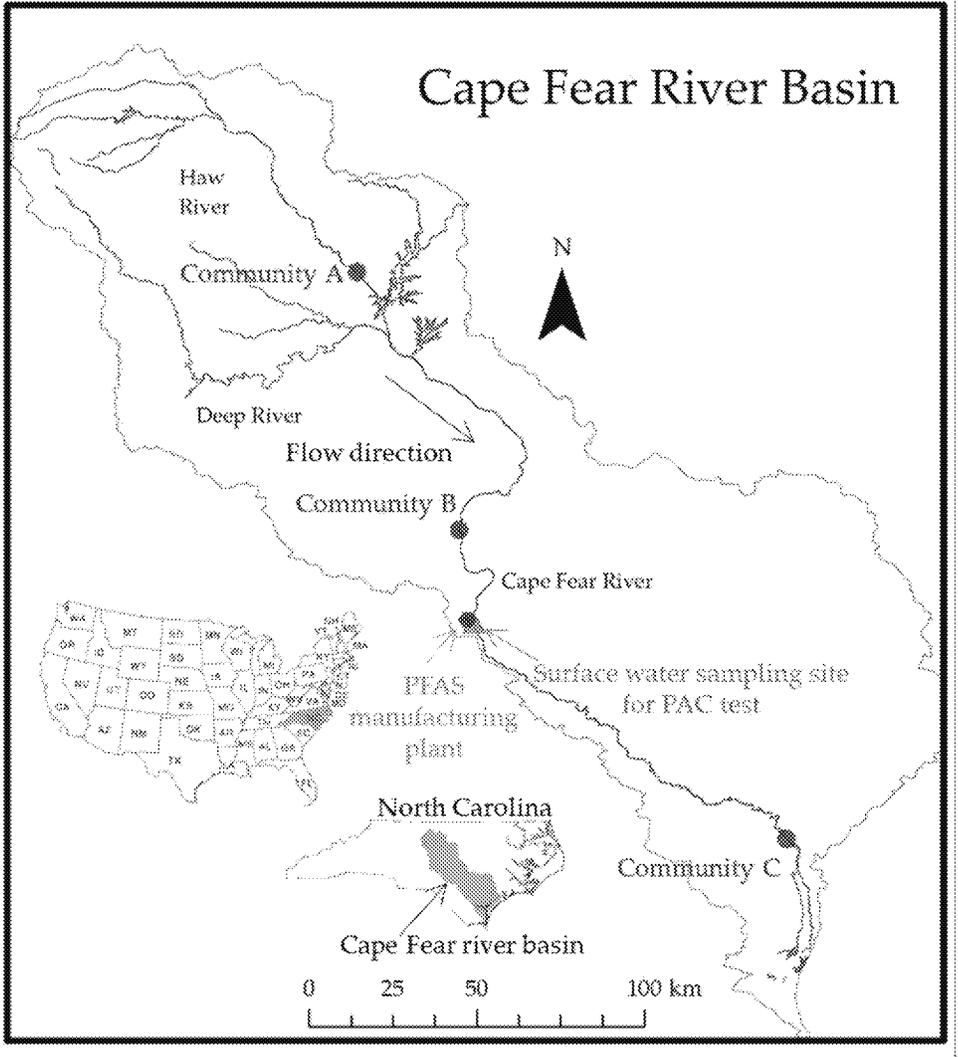
	Compound	MS/MS Transition	Internal standard
Traditional PFASs	PFBA	212.8 > 168.8	13C4-PFBA
	PFPeA	262.9 > 218.8	13C2- PFHxA
	PFHxA	313.6 > 268.8	13C2- PFHxA
	PFHpA	362.9 > 318.8	13C4- PFOA
	PFOA	413.0 > 368.8	13C4- PFOA
	PFNA	463.0 > 418.8	13C4- PFOA
	PFDA	513.1 > 468.8	13C2-PFDA
	PFBS	299.1 > 98.8	18O2-PFHxS
	PFHxS	399.1 > 98.8	18O2-PFHxS
	PFOS	498.9 > 98.8	13C4-PFOS
PFECAs	PFMOAA	180.0 > 85.0	N/A
	PFMOPrA	229.1 > 184.9	N/A
	PFMOBA	279.0 > 234.8	N/A
	PFPrOPrA	330.0 > ?	13C2- PFHxA
	PFO2HxA	245.1 > 85.0	N/A
	PFO3OA	311. > 84.9	N/A
	PFO4DA	377.1 > 85.0	N/A
Internal standards	Perfluoro-n-[1,2,3,4- ¹³ C ₄]butanoic acid (13C4-PFBA)	217.0 > 172	Not applicable
	Perfluoro-n-[1,2- ¹³ C ₂]hexanoic acid (13C2-PFHxA)	315.1 > 269.8	
	Perfluoro-n-[1,2,3,4- ¹³ C ₂]octanoic acid (13C4-PFOA)	415.0 > 369.8	
	Perfluoro-n-[1,2- ¹³ C ₂]decanoic acid (13C2-PFDA)	515.1 > 469.8	
	Sodium perfluoro-1-hexane[¹⁸ O ₂]sulfonate (18O2-PFHxS)	403.1 > 83.8	
	Sodium perfluoro-1-[1,2,3,4- ¹³ C ₄]octane sulfonate (13C4-PFOS)	502.9 > 79.9	

Table S4. Maximum, minimum, mean and median concentrations (ng/L) of PFASs in CFR watershed surface water as drinking water sources. *

	Community A				Community B				Community C			
	max	min	median	mean	max	min	median	mean	max	min	median	mean
PFBA	99	<10	26	33	38	<10	12	12	104	<10	12	22
PFPeA	191	14	44	62	38	<10	19	19	116	<10	30	36
PFHxA	318	<10	48	78	42	<10	<10	11	24	<10	<10	<10
PFHpA	324	<10	39	67	85	<10	<10	11	24	<10	<10	<10
PFOA	137	<10	34	46	32	<10	<10	<10	17	<10	<10	<10
PFNA	38	<10	<10	<10	<10	<10	<10	<10	<10	<10	<10	<10
PFDA	35	<25	<25	<25	<25	<25	<25	<25	<25	<25	<25	<25
PFBS	80	<10	<10	<10	11	<10	<10	<10	<10	<10	<10	<10
PFHxS	193	<10	10	14	14	<10	<10	<10	14	<10	<10	<10
PFOS	346	<25	29	44	43	<25	<25	<25	40	<25	<25	<25
PFPrOPrA	<10	<10	<10	<10	10	<10	<10	<10	4560	55	304	631
∑ PFASs**	1502	18	212	355	189	0	47	62	4560	55	304	631

* Concentrations < quantification limits were considered as zero to calculate means and ∑ PFASs.

** Other PFECAs were present in water samples from community C but could not be quantified and were therefore not included in ∑ PFASs



Commented [SJ1]: This belongs in the main text as it is central to the comparisons of the communities.

Figure S2. Sampling sites in Cape Fear River watershed, North Carolina

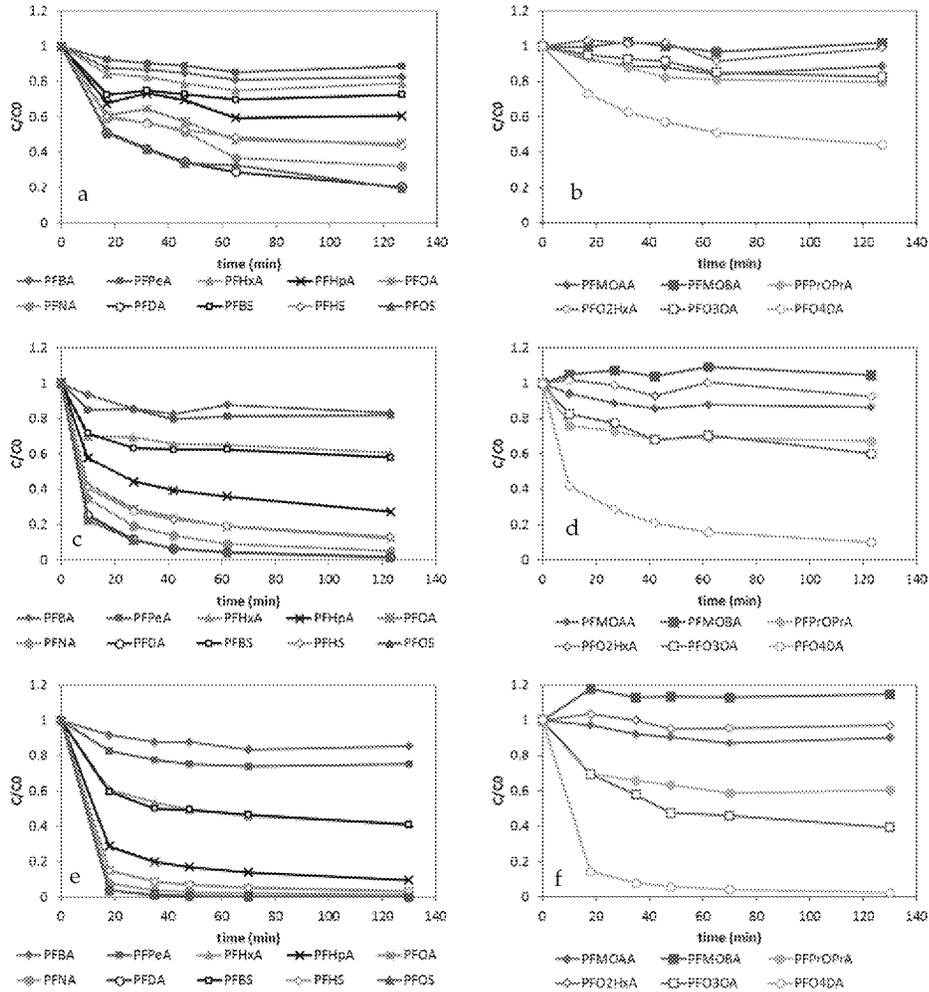


Figure S3. PFAS adsorption to PAC at carbon doses of (a, b) 30 mg/L, (c, d) 60 mg/L and (e, f) 100 mg/L. The chart shows the average of remaining PFAS percentage of duplicate tests.